

# Upper critical field in layered superconductors

V.P.Mineev<sup>1,2</sup>

<sup>1</sup> *Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto 606-8502, Japan*

<sup>2</sup> *Commissariat a l'Energie Atomique, Departement de Recherche Fondamentale sur la Matiere Condensee, SPSMS, 38054, Grenoble, France*

(Submitted 23 February 2000)

The theoretical statements about a restoration of a superconductivity at magnetic fields higher than the quasiclassical upper critical field and a reentrance of superconductivity at temperatures  $T_c(H) \approx T_c(0)$  in the superconductors with open Fermi surfaces are reinvestigated taking into account a scattering of quasiparticles on the impurities.

The system of integral equations for determination of the upper critical field parallel to the conducting planes in a layered conventional and unconventional superconductors with impurities are derived. The  $H_{c2}(T)$  values for the "clean" case in the Ginzburg-Landau regime and at any temperature in the "dirty" case are found analytically. The upper limit of the superconductor purity when the upper critical field definitely has a finite value is established.

KEYWORDS: anisotropic superconductivity, upper critical field,  $Sr_2RuO_4$ .

## I. INTRODUCTION

The theory of upper critical field in highly anisotropic quasi-two-dimensional superconductors for the field orientation parallel to conducting layers has been developed by A. Lebed' and K. Yamaji<sup>1</sup>. It was shown that like in quasi-one-dimensional case<sup>2</sup> at low enough temperatures (see below) the upper critical field starts to diverge such that a superconductivity is conserved in arbitrary large magnetic fields. Moreover in high enough magnetic fields (see below) the critical temperature of a superconducting phase transition has a tendency to restore of its zero field value. These statements are literally true for the superconductors with triplet pairing. For a singlet pairing the existence of a superconductivity in high fields is restricted by the paramagnetic limit  $H_p$ . So, the low temperature stability of a superconducting state under magnetic field can serve as the indication on the superconductivity with triplet pairing.

The tendency for low temperature divergence of the upper critical field  $H_{c2} > H_p$  in quasi-two-dimensional  $\kappa$ -type ET organic superconductors has been reported recently by T. Ishiguro<sup>3</sup>. Similar behavior has been observed earlier in quasi-one-dimensional organic superconductor  $(TMTSF)_2PF_6$  by the group of P. Chaikin<sup>4</sup>. So, the observations being in correspondence with theoretical predictions<sup>1,2</sup> say in favor of triplet type of superconductivity in both type of these materials.

Another popular layered superconductor is  $Sr_2RuO_4$ . It demonstrates the properties compatible with triplet superconductivity<sup>5</sup>. Unlike isostructural high- $T_c$  cuprates  $La_{2-x}Ba_xCuO_4$  the normal state of layered perovskite oxide  $Sr_2RuO_4$  conforms with the predictions of Fermi-liquid theory<sup>6</sup>. Unconventional nature of the superconducting state in this material manifests itself through the strong suppression of  $T_c$  by nonmagnetic impurities<sup>7,8</sup> as well as by the exhibition of a sharp decrease without the coherence peak of  $^{101}Ru$  nucleare spin-relaxation rate  $1/T_1$  followed by  $T^3$  behavior down to  $0.15K$ <sup>9</sup>. The spin part of  $^{17}O$  Knight shift for the field  $H = 0.65T$  parallel to  $ab$  plane does not change down to  $15mK$ , much below  $T_c(H) \approx 1.2K$ <sup>10</sup>. Since the experiment has been performed on  $Sr_2RuO_4$  in a clean limit this constitutes the evidence for the triplet spin pairing with spin of pairs lying in  $ab$  plane. On the other hand the measurements of the basal plane upper critical field down to  $0.2K$  shows no tendency to divergency of  $H_{c2}(T)$ <sup>11</sup> (see also results of measurements on less perfect crystals<sup>12</sup>). Moreover, the search for reentrance of superconductivity under magnetic fields up to  $33T$  and temperatures down to  $50$  mK has given the negative results<sup>13</sup>. The basal plane upper critical field saturates at low temperatures at  $1.5T$  which is well below the paramagnetic limit  $H_p \approx 2.8T$  and roughly corresponds to quasiclassical upper critical field value

$$H_{c2} = \frac{\Phi_0}{2\pi\xi_{ab}\xi_c}, \quad (1)$$

where  $\Phi_0$  is the flux quantum and  $\xi_{ab}$ ,  $\xi_c$  are the coherence lengths in basal plane and along the  $c$  axis correspondingly.

These observations being certainly in contradiction with theory<sup>1</sup> stimulate us to reinvestigate the problem of upper critical field in quasi-two-dimensional superconductors taking into account scattering of quasiparticles on the impurities. The main goal is to find a limits for crystal purity when one can hope to see the low temperature upper critical field divergency. In a few words the result can be described as follows. In a pure crystal the  $H_{c2}$  divergency starts to be developed when the thermal coherence length  $\xi(T) = v_F/2\pi T$  begins to be larger than the "cyclotron radius" of the quasiparticles orbits  $R_c(H) = v_F/\omega_c$ . Here  $v_F$  is the basal plane Fermi velocity,  $\omega_c = eHv_Fd/c$  is the "cyclotron frequency",  $d$  is the distance between conducting layers. The impurities does not prevent the upper critical field divergency if at the temperature determined by equality

$$\xi(T) = R_c(H_{c2}) \quad (2)$$

the quasiparticles mean free path  $l$  is still larger than  $\xi(T)$ . Otherwise the upper critical field is saturated at temperatures below

$$T_l = \frac{v_F}{2\pi l} \quad (3)$$

and its value is roughly described by formula (1).

The paper has following structure. The general formalism for the upper critical field problem in layered conventional and unconventional superconductors is introduced in the next Section. By the way of the derivation the several simplifications have been used: (i) The equations are written for axially symmetric crystal where the only one-dimensional, even or odd in respect to the reflections in ( $\mathbf{H}$ , crystal axis) plane superconducting states are realized; (ii) Among them the only even superconducting states are considered; (iii) The equations are derived with but solved in neglect Pauli paramagnetic interaction; (iv) The equations are solved for only unconventional superconducting states with zero anomalous Green function self-energy. The analytical solution of the equations accompanied by the discussion of limits of crystal purity sufficient for the upper critical field saturation at low temperature is contained in the third Section.

## II. THE ORDER PARAMETER EQUATIONS

The electron spectrum of a layered crystals obeys basal plane anisotropy,  $z$ -dependent corrugation of the Fermi surface and several bands in general case. It seems however unimportant for our purposes to take into account all these complications. So, we shall consider a metal with electron spectrum

$$\begin{aligned}\epsilon(\mathbf{p}) &= \frac{1}{2m}(p_x^2 + p_y^2) - 2t \cos p_z d, \\ t \ll \epsilon_F &= \frac{mv_F^2}{2}, \quad -\frac{\pi}{d} < p_z < \frac{\pi}{d}\end{aligned}\quad (4)$$

in the magnetic field  $\mathbf{H} = (0, H, 0)$ ,  $\mathbf{A} = (0, 0, -Hx)$  parallel to the conducting layers with distance  $d$  between them. In absence of impurities the normal state electron Green function  $G_{\omega_n, \sigma}(p_y, p_z, x, x')$  is obtained as the result of solution of the equation

$$\left[ i\omega - \frac{1}{2m} \left( -\frac{d^2}{dx^2} + p_y^2 \right) + 2t \cos \left( p_z d - \frac{\omega_c x}{v_F} \right) + \sigma \mu_e H + \mu \right] G_{\omega, \sigma}(p_y, p_z, x, x') = \delta(x - x'), \quad (5)$$

where  $\omega_n = \pi T(2n + 1)$  is the Matsubara frequency,  $\omega_c = ev_F dH/c$ ,  $v_F$  is the Fermi velocity,  $\hbar = 1$ ,  $\mu$  is the chemical potential,  $\mu_e$  is a magnetic moment of an electron in a crystal. To use the diagonal shape of the Green function matrix we have chosen the  $\hat{y}$  direction as the spin quantization axis, such that  $\sigma = \pm 1$ .

In a layered crystal with a singlet Cooper pairing the superconducting states obey the following order parameters

$$\hat{\Delta}^s = i\Delta^s(p_x, p_y, p_z, x)\hat{\sigma}_y, \quad (6)$$

Here,  $\hat{\sigma}_y$  is the Pauli matrix. For a triplet superconductivity we shall limit ourselves by the consideration of the so called equal spin pairing states with spin lying in the plane of the conducting layers. In neglect of small effects of spontaneous magnetism<sup>14</sup> a vector wave function of such the states is

$$\mathbf{d} = \hat{z}\Delta^t(p_x, p_y, p_z, x). \quad (7)$$

As we have put the spin quantization axis along  $\hat{y}$  direction we will use the corresponding basis of Pauli matrices  $\vec{\sigma} = (\hat{\sigma}_y, \hat{\sigma}_z, \hat{\sigma}_x)$ . So the order parameter for triplet pairing state in our case is

$$\hat{\Delta}^t = i(\mathbf{d}\vec{\sigma})\sigma_y = -\Delta^t(p_x, p_y, p_z, x)\hat{\sigma}_z. \quad (8)$$

The order parameter function is represented<sup>15</sup> as a linear combination of the basis functions  $\psi_i(\phi, p_z)$  of one of the irreducible representations of crystal symmetry group

$$\Delta^{s,t}(p_x, p_y, p_z, x) = \psi_i(\phi, p_z)\Delta^{s,t}_i(x). \quad (9)$$

Here,  $\phi$  is the angle between basal plane vector of momentum  $\mathbf{p}_{\parallel}$  and magnetic field  $\mathbf{H} \parallel \hat{y}$ . There are only one and two dimensional representations ( $i = 1, \dots, d; d = 1, 2$ ) in the crystals with axially symmetric spectrum (4).

The crystal with axial symmetry under magnetic field lying in the basal plane obeys the symmetry in respect of reflections in plane where the vectors of magnetic field and crystal axis lie, that is  $(y, z)$  plane in our case <sup>1</sup>. The two components of vector basis functions  $(\psi_1(\phi, p_z), \psi_2(\phi, p_z))$  can be always chosen such that each of them will have definite (even or odd) and at the same time mutually opposite parity in respect to reflections in  $(y, z)$  plane. As the consequence the set of the order parameter equations for two component superconductivity splits on two independent equation for each component of the order parameter. One of them corresponds to the higher value of the upper critical field. Thus we always deal with one-component superconductivity with definite parity. The simplest examples of even functions  $\psi(\phi, p_z)$  are:  $1, \sin^2 \phi - \cos^2 \phi$  for singlet pairing and  $\sin(p_z d), \cos \phi$  for triplet pairing. As an examples of odd states one can pointed out on  $\sin(p_z d) \sin \phi$  for singlet pairing and  $\sin \phi$  for the triplet pairing.

The upper critical field is found from the equation on the order parameter which have the different shape for even and odd superconducting states. For determiness we shall consider just the even order parameter states. In this case the order parameter equation for a clean superconductor with singlet pairing is

$$\begin{aligned} \Delta^s(\phi, p_z, x) = & g \int dx' \int \frac{dp'_y}{2\pi} \int_{-\pi/d}^{\pi/d} \frac{dp'_z}{2\pi} \psi(\phi, p_z) \psi^*(\phi', p'_z) \\ & \times T \sum_n \frac{1}{2} \sum_{\sigma=\pm 1} G_{\omega_n, \sigma}(p'_y, p'_z, x, x') G_{-\omega_n, -\sigma}(-p'_y, -p'_z, x, x') \Delta^s(\phi', p'_z, x') \end{aligned} \quad (10)$$

and for the triplet pairing

$$\begin{aligned} \Delta^t(\phi, p_z, x) = & g \int dx' \int \frac{dp'_y}{2\pi} \int_{-\pi/d}^{\pi/d} \frac{dp'_z}{2\pi} \psi(\phi, p_z) \psi^*(\phi', p'_z) \\ & \times T \sum_n \frac{1}{2} \sum_{\sigma=\pm 1} G_{\omega_n, \sigma}(p'_y, p'_z, x, x') G_{-\omega_n, \sigma}(-p'_y, -p'_z, x, x') \Delta^t(\phi', p'_z, x') \end{aligned} \quad (11)$$

In presence of the impurities the order parameter of a superconducting singlet pairing state  $\hat{\Delta}^s = i\Delta^s(\phi, p_z, x)\hat{\sigma}_y$  acquires a self energy part

$$\hat{\Sigma}^s(\omega_n, x) = i\Delta_{\omega_n}^s(x)\hat{\sigma}_y + \Delta_{\omega_n}^t(x)\hat{\sigma}_x \quad (12)$$

consisting of singlet and triplet components <sup>2</sup>

For a triplet pairing states with an order parameter  $\hat{\Delta}^t = -\Delta^t(\phi, p_z, x)\hat{\sigma}_z$  the corresponding self energy part

$$\hat{\Sigma}^t(\omega_n, x) = -\Delta_{\omega_n}^t(x)\hat{\sigma}_z + i\tilde{\Delta}_{\omega_n}^t(x)\hat{\sigma}_0 \quad (13)$$

consists of two different triplet components. Here  $\hat{\sigma}_0$  is the two dimensional unit matrix. The singlet component of self energy part is absent for chosen basal plane orientation of magnetic field and equal spin triplet pairing with spin directions parallel to conducting layers.

The self-consistency equations for the order parameters and self energy parts have the form (see<sup>15</sup>)

$$\Delta_{\alpha\beta}^{s,t} = \int dx' \int \frac{dp'_y}{2\pi} \int_{-\pi/d}^{\pi/d} \frac{dp'_z}{2\pi} V_{\beta\alpha, \lambda\mu}^{s,t}$$

---

<sup>1</sup>For the uniaxial crystals with hexagonal or tetragonal symmetry this property takes place only for particular directions of magnetic field in the basal plane.

<sup>2</sup>Compare with the paper<sup>16</sup>, where a similar theory in frame of quasiclassical approach has been developed.

$$\begin{aligned}
& \times T \sum_n G_{\tilde{\omega}_n}^{\lambda\gamma}(p'_y, p'_z, x, x') G_{-\tilde{\omega}_n}^{\mu\delta}(-p'_y, -p'_z, x, x') [\Delta^{s,t}_{\gamma\delta}(\phi', p'_z, x') + \Sigma^{s,t}_{\gamma\delta}(\tilde{\omega}_n, x')], \\
& \Sigma_{\gamma\delta}^{s,t}(\tilde{\omega}_n, x) = nu^2 \int dx' \int \frac{dp'_y}{2\pi} \int_{-\pi/d}^{\pi/d} \frac{dp'_z}{2\pi} \\
& \times G_{\tilde{\omega}_n}^{\gamma\alpha}(p'_y, p'_z, x, x') G_{-\tilde{\omega}_n}^{\beta\delta}(-p'_y, -p'_z, x, x') [\Delta^{s,t}_{\alpha\beta}(\phi', p'_z, x') + \Sigma^{s,t}_{\alpha\beta}(\tilde{\omega}_n, x')], \tag{14}
\end{aligned}$$

where  $V_{\beta\alpha, \lambda\mu}^{s,t} = g g^{s,t}_{\beta\alpha} g^{s,t}_{\lambda\mu} \psi(\phi, p_z) \psi^*(\phi', p'_z)/2$ ,  $\hat{g}^s = i\hat{\sigma}_y$ ,  $\hat{g}^t = -\hat{\sigma}_z$ ;

$G_{\tilde{\omega}_n}^{\lambda\gamma} = G_{\tilde{\omega}_n,1}(\sigma_0^{\lambda\gamma} + \sigma_z^{\lambda\gamma})/2 + G_{\tilde{\omega}_n,-1}(\sigma_0^{\lambda\gamma} - \sigma_z^{\lambda\gamma})/2$ .

Here  $\tilde{\omega}_n = \omega_n + \Gamma \text{sign}\omega_n$ ,  $\Gamma = mn u^2/2d$  and  $u, n$  are impurity potential amplitude and concentration. We will use also a quasiparticle life time  $\tau$  and a mean free path  $l$  introduced by means  $\Gamma = 1/2\tau = v_F/2l$ .

The equations (14) are obtained in frame of procedure of averaging over an impurity positions. As it was shown in the paper<sup>17</sup> one can use the field independent value of  $\Gamma$  so long

$$\frac{v_F}{\omega_c} > \frac{l}{\sqrt{k_F l}}. \tag{15}$$

The system of "the scalar" self-consistency equations for the singlet pairing states following of equations (14) is

$$\begin{aligned}
& \Delta^s(\phi, p_z, x) = g \int dx' \int \frac{dp'_y}{2\pi} \int_{-\pi/d}^{\pi/d} \frac{dp'_z}{2\pi} \psi(\phi, p_z) \psi^*(\phi', p'_z) \\
& \times T \sum_n \frac{1}{2} \sum_{\sigma=\pm 1} G_{\tilde{\omega}_n, \sigma}(p'_y, p'_z, x, x') G_{-\tilde{\omega}_n, -\sigma}(-p'_y, -p'_z, x, x') [\Delta^s(\phi', p'_z, x') + \Delta_{\tilde{\omega}_n}^s(x') + \sigma \Delta_{\tilde{\omega}_n}^t(x')], \tag{16}
\end{aligned}$$

$$\begin{aligned}
& \Delta_{\tilde{\omega}_n}^s(x) = nu^2 \int dx' \int \frac{dp_y}{2\pi} \int_{-\pi/d}^{\pi/d} \frac{dp_z}{2\pi} \frac{1}{2} \sum_{\sigma=\pm 1} G_{\tilde{\omega}_n, \sigma}(p_y, p_z, x, x') G_{-\tilde{\omega}_n, -\sigma}(-p_y, -p_z, x, x') \\
& \times [\Delta^s(\phi, \hat{p}_z, x') + \Delta_{\tilde{\omega}_n}^s(x') + \sigma \Delta_{\tilde{\omega}_n}^t(x')], \tag{17}
\end{aligned}$$

$$\begin{aligned}
& \Delta_{\tilde{\omega}_n}^t(x) = nu^2 \int dx' \int \frac{dp_y}{2\pi} \int_{-\pi/d}^{\pi/d} \frac{dp_z}{2\pi} \frac{1}{2} \sum_{\sigma=\pm 1} G_{\tilde{\omega}_n, \sigma}(p_y, p_z, x, x') G_{-\tilde{\omega}_n, -\sigma}(-p_y, -p_z, x, x') \\
& \times [\sigma(\Delta^s(\phi, \hat{p}_z, x') + \Delta_{\tilde{\omega}_n}^s(x')) + \Delta_{\tilde{\omega}_n}^t(x')]. \tag{18}
\end{aligned}$$

For the triplet pairing case the corresponding equations are

$$\begin{aligned}
& \Delta^t(\phi, p_z, x) = g \int dx' \int \frac{dp'_y}{2\pi} \int_{-\pi/d}^{\pi/d} \frac{dp'_z}{2\pi} \psi(\phi, p_z) \psi^*(\phi', p'_z) \\
& \times T \sum_n \frac{1}{2} \sum_{\sigma=\pm 1} G_{\tilde{\omega}_n, \sigma}(p'_y, p'_z, x, x') G_{-\tilde{\omega}_n, \sigma}(-p'_y, -p'_z, x, x') [\Delta^t(\phi', p'_z, x') + \Delta_{\tilde{\omega}_n}^t(x') - i\sigma \tilde{\Delta}_{\tilde{\omega}_n}^t(x')], \tag{19}
\end{aligned}$$

$$\begin{aligned}
& \Delta_{\tilde{\omega}_n}^t(x) = nu^2 \int dx' \int \frac{dp_y}{2\pi} \int_{-\pi/d}^{\pi/d} \frac{dp_z}{2\pi} \frac{1}{2} \sum_{\sigma=\pm 1} G_{\tilde{\omega}_n, \sigma}(p_y, p_z, x, x') G_{-\tilde{\omega}_n, \sigma}(-p_y, -p_z, x, x') \\
& \times [\Delta^t(\phi, p_z, x') + \Delta_{\tilde{\omega}_n}^t(x') - i\sigma \tilde{\Delta}_{\tilde{\omega}_n}^t(x_1)], \tag{20}
\end{aligned}$$

$$\begin{aligned} \tilde{\Delta}_{\tilde{\omega}_n}^t(x) = nu^2 \int dx' \int \frac{dp_y}{2\pi} \int_{-\pi/d}^{\pi/d} \frac{dp_z}{2\pi} \frac{1}{2} \sum_{\sigma=\pm 1} G_{\tilde{\omega}_n, \sigma}(p_y, p_z, x, x') G_{-\tilde{\omega}_n, \sigma}(-p_y, -p_z, x, x') \\ \times [i\sigma(\Delta^t(\phi, p_z, x') + \Delta_{\tilde{\omega}_n}^t(x')) + \tilde{\Delta}_{\tilde{\omega}_n}^t(x')]. \end{aligned} \quad (21)$$

Taking into account that in common the paramagnetic limit of superconductivity  $H_p$  is much higher than an orbital upper critical field we shall rest the general problem of influence of paramagnetism on superconductivity for a future investigations. In the absence of the Pauli paramagnetic interaction the equations (16)-(21) are greatly simplified and we have the system of two equations with equivalent structure for singlet and triplet pairing states

$$\begin{aligned} \Delta^{s,t}(\phi, p_z, x) = g \int dx' \int \frac{dp'_y}{2\pi} \int_{-\pi/d}^{\pi/d} \frac{dp'_z}{2\pi} \psi(\phi, p_z) \psi^*(\phi', p'_z) \\ \times T \sum_n G_{\tilde{\omega}_n}(p'_y, p'_z, x, x') G_{-\tilde{\omega}_n}(-p'_y, -p'_z, x, x') (\Delta^{s,t}(\phi', p'_z, x') + \Delta_{\tilde{\omega}_n}^{s,t}(x')), \end{aligned} \quad (22)$$

$$\begin{aligned} \Delta_{\tilde{\omega}_n}^{s,t}(x) = nu^2 \int dx' \int \frac{dp_y}{2\pi} \int_{-\pi/d}^{\pi/d} \frac{dp_z}{2\pi} \\ \times G_{\tilde{\omega}_n}(p_y, p_z, x, x') G_{-\tilde{\omega}_n}(-p_y, -p_z, x, x') (\Delta^{s,t}(\phi, \hat{p}_z, x') + \Delta_{\tilde{\omega}_n}^{s,t}(x')). \end{aligned} \quad (23)$$

Below we shall omit the supercripts  $s, t$  using the common notation  $\Delta^{s,t}(\phi, p_z, x) = \Delta(\phi, p_z, x)$ ,  $\Delta_{\tilde{\omega}_n}^{s,t}(x) = \Delta_{\tilde{\omega}_n}(x)$  for the order parameters and the self energy parts both in singlet and in triplet case.

On this stage it is useful to note that the normal metal electron Green function which we should find as a solution of the equation (5) depends of  $p_y$  only through its square. Hence for some unconventional superconducting phases like  $\Delta(\phi, \hat{p}_z, x) = \sqrt{2}(\sin^2 \phi - \cos^2 \phi) \Delta(x)$  for singlet pairing or  $\Delta(\phi, \hat{p}_z, x) = \sqrt{2} \cos \phi \Delta(x)$  for triplet pairing, the following property takes place

$$\int \frac{dp_y}{2\pi} G_{\tilde{\omega}_n}(p_y, p_z, x, x') G_{-\tilde{\omega}_n}(-p_y, -p_z, x, x') (\Delta(\phi, \hat{p}_z, x) = 0. \quad (24)$$

We will discuss further the only unconventional superconducting states obeying the property (24). For such the states the self energy part is equal to zero and we deal only with the order parameter equation.

$$\begin{aligned} \Delta(\phi, p_z, x) = g \int dx' \int \frac{dp'_y}{2\pi} \int_{-\pi/d}^{\pi/d} \frac{dp'_z}{2\pi} \psi(\phi, p_z) \psi^*(\phi', p'_z) \\ \times T \sum_n G_{\tilde{\omega}_n}(p'_y, p'_z, x, x') G_{-\tilde{\omega}_n}(-p'_y, -p'_z, x, x') \Delta(\phi', p'_z, x'). \end{aligned} \quad (25)$$

The equality (24) is not valid for conventional superconducting state as well for many unconventional superconducting states where, as the consequence, there are nonzero selfenergy parts. In isotropic conventional superconducting state it prevents a suppression of the superconductivity by the ordinary impurities. For unconventional superconducting states the presence of the self energy leads just to the mathematical complications and does not change qualitatively the main results.

The only difference of (25) from the pure case consists of change  $\omega_n \rightarrow \tilde{\omega}_n$  and one can use the expression for the normal metal electron Green function found in the paper<sup>1</sup>. It has nonzero value in the regions determined by the inequality  $\omega_n(x - x_1) \geq 0$  for positive value of  $x$  component of electron momentum ( $\alpha = 1$ ) and by the inequality  $\omega_n(x - x_1) \leq 0$  for negative values of  $x$  component momentum ( $\alpha = -1$ ), where it is defined as

$$G_{\tilde{\omega}_n}(\phi, p_z, x, x_1) = \frac{-i \text{sign} \omega_n}{v_F \sin \phi} \exp \left[ -\frac{\alpha \tilde{\omega}_n (x - x_1)}{v_F \sin \phi} \right] \exp[i\alpha p_F (x - x_1) \sin \phi] \\ \times \exp \left\{ \frac{i\alpha \lambda}{\sin \phi} \sin \left[ \frac{\omega_c (x - x_1)}{2v_F} \right] \cos \left[ p_z d - \frac{\omega_c (x + x_1)}{2v_F} \right] \right\}. \quad (26)$$

Here  $\lambda = 4t/\omega_c$ .

This expression is valid under the condition

$$|\sin \phi| > \sqrt{\frac{t}{\epsilon_F}}. \quad (27)$$

The disregard of the small intervals of the angle  $\phi$  where  $|\sin \phi| < (t/\epsilon_F)^{1/2}$  means that the only open trajectories of quasiparticles on the Fermi surface are taken into account<sup>3</sup> They give the main singular part to the kernels of the integral equation (25).

The substitution of (26) to the equation (27) gives after summation over the Matsubara frequency

$$\Delta(x) = \tilde{g} \int_{|x-x_1|>a}^{\pi} dx_1 \int_0^{\pi} \frac{d\phi}{2\pi v_F \sin \phi} \int_{-\pi}^{\pi} \frac{d(p_z d)}{2\pi} \psi^*(\phi, p_z) \psi(\phi, p_z) \frac{2\pi T \exp \left[ -\frac{|x-x_1|}{t \sin \phi} \right]}{\sinh \left[ \frac{2\pi T |x-x_1|}{v_F \sin \phi} \right]} \\ \times \exp \left\{ \frac{2i\lambda}{\sin \phi} \sin \left[ \frac{\omega_c (x - x_1)}{2v_F} \right] \sin(p_z d) \sin \left[ \frac{\omega_c (x + x_1)}{2v_F} \right] \right\} \Delta(x_1). \quad (28)$$

Here  $\tilde{g} = gm/4\pi d$  is dimensionless constant of pairing interaction,  $a$  is the small distances cutoff. The equation (28) is the basic equation of the paper. The properties of its solution we shall discuss in the next Section.

### III. THE UPPER CRITICAL FIELD

Let us make an unessential simplification and consider  $p_z$  independent superconducting states determined by functions  $\psi(\phi)$  normalized as follows

$$\int_0^{\pi} \frac{d\phi}{\pi} \psi^*(\phi) \psi(\phi) = 1.$$

In this case one can perform the integration over  $p_z$  in (28):

$$\Delta(x) = \tilde{g} \int_{|x-x_1|>a}^{\pi} dx_1 \int_0^{\pi} \frac{d\phi}{2\pi v_F \sin \phi} \psi^*(\phi) \psi(\phi) \frac{2\pi T \exp \left[ -\frac{|x-x_1|}{t \sin \phi} \right]}{\sinh \left[ \frac{2\pi T |x-x_1|}{v_F \sin \phi} \right]} \\ \times \mathcal{I}_0 \left\{ \frac{2\lambda}{\sin \phi} \sin \left[ \frac{\omega_c (x - x_1)}{2v_F} \right] \sin \left[ \frac{\omega_c (x + x_1)}{2v_F} \right] \right\} \Delta(x_1). \quad (29)$$

Here  $\mathcal{I}_0(\dots)$  is the Bessel function. For the further purposes it is not important to work with the equation (28) or with (29) and for the determineness we will operate with the latter.

The equation (29) in the absence of a magnetic field

---

<sup>3</sup> The numerical calculation taking into account both open and closed trajectories, performed for clean case in the paper<sup>18</sup>, just confirms the qualitative results of the article<sup>1</sup> have been obtained in neglect of closed trajectories.

$$1 = \tilde{g} \int_{\frac{2\pi a T}{v_F}}^{\infty} \frac{dz}{\sinh z} \exp\left(-\frac{z}{2\pi T \tau}\right) \quad (30)$$

determines of the critical temperature  $T_c$ , which is expressed from here through the critical temperature  $T_{c0}$  in a perfect crystal without impurities  $l = \infty$

$$T_{c0} = \frac{v_F}{\pi a} \exp\left(-\frac{1}{\tilde{g}}\right) \quad (31)$$

by means of well known relation

$$\ln \frac{T_c}{T_{c0}} = \psi\left(\frac{1}{2}\right) - \psi\left(\frac{1}{2} + \frac{1}{4\pi\tau T_c}\right). \quad (32)$$

For the critical temperatures  $T_c \sim T_{c0}$  the suppression of the superconductivity by the impurities is:

$$T_c = T_{c0} - \frac{\pi}{8\tau}. \quad (33)$$

One can also point out the condition of complete suppression of the superconductivity

$$\tau = \tau_c = \frac{\gamma}{\pi T_{c0}}, \quad (34)$$

where  $\ln \gamma = C = 0,577\dots$  is the Euler constant.

The behavior of the upper critical field is determined by the relationship of the three spacial scales:  $v_F/2\pi T$ ,  $l$  and  $v_F/\omega_c$ . For the temperatures near to the zero field critical temperature  $T \approx T_c(H = 0)$  the upper critical field  $H_{c2}(T)$ , or  $\omega_{c2}(T) = eH_{c2}(T)v_F d/c$  tends to zero and the inequality

$$\min\left\{\frac{v_F}{2\pi T}, l\right\} < \frac{v_F}{\omega_{c2}(T)} \quad (35)$$

always presents <sup>4</sup>.

At the temperature decrease the upper critical field increase, but so long the inequality (35) takes place the essential interval of integration over  $(x - x_1)$  in (29) determined by the  $\min(v_F/2\pi T, l)$ . Hence, one can use the smallness of  $(x - x_1)v_F/\omega_c$  in the kernel of the equation (29):

$$\Delta(x) = \tilde{g} \int_{|x-x_1| > a \sin \phi} dx_1 \int_0^{\pi} \frac{d\phi}{2\pi v_F \sin \phi} \psi^*(\phi) \psi(\phi) \frac{2\pi T \exp\left[-\frac{|x-x_1|}{l \sin \phi}\right]}{\sinh\left[\frac{2\pi T |x-x_1|}{v_F \sin \phi}\right]} \mathcal{I}_0\left\{\frac{4t(x-x_1)}{v_F \sin \phi} \sin \frac{\omega_c x}{v_F}\right\} \Delta(x_1). \quad (36)$$

The solution of this equation gives the correct value of  $\omega_{c2}(T)$  so long the inequality (35) is truth. By the substitution of the  $\omega_{c2}(T)$  obtained from this equation to the inequality (35) one can establish the upper limit of the superconductor purity at which the  $H_{c2}(T)$  found from this equation represent the correct value of the upper critical field up to zero temperature.

For the pure enough samples and low enough temperatures it can be turn out that the opposite to the (35) relationship

$$\frac{v_F}{\omega_{c2}(T)} < \min\left\{\frac{v_F}{2\pi T}, l\right\} \quad (37)$$

---

<sup>4</sup>Near  $T_c$  there is also formal solution of (29) with  $\omega_{c2} > t$  (see<sup>1</sup>). This solution, however, is related to the region of magnetic fields, out the region of validity of the present theory (15).



breaking the correctness of transferring from (29) to (36) is realized. It should be noted that ultraclean case demands a special investigation (see condition (15) and discussion in the paper<sup>17</sup>). One can claim however, that at the temperatures

$$\frac{v_F}{2\pi l} < T < \frac{\omega_c(T)}{2\pi}$$

the magnetic field dependence of the critical temperature in the equation (29) starts disappear or, in other words, the tendency to the divergency of the upper critical field pointed out in the paper<sup>1</sup> appears.

To solve of the equation (36) at arbitrary temperature and purity is possible only numerically. Here we shall discuss the case when it allows the analitical solution. If the legth scale  $\xi$ , on which the function  $\Delta(x)$  is localized, is larger than the essential distance of integration over  $(x - x_1)$

$$\xi > \min \left\{ \frac{v_F}{2\pi T}, l \right\}, \quad (38)$$

then one can expand  $\Delta(x_1) \approx \Delta(x) + \Delta'(x)(x - x_1) + \Delta''(x)(x - x_1)^2/2$  under the integral in (36). Taking into consideration that under this condition the argument of Bessel function turns to be small even on the upper boundary of effective interval of the integration over  $(x - x_1)$ :

$$\frac{t\omega_{c2}(T)\xi \min \left\{ \frac{v_F}{2\pi T}, l \right\}}{v_F^2} \approx \frac{t \min \left\{ \frac{v_F}{2\pi T}, l \right\}}{\epsilon_F \xi} < 1, \quad (39)$$

one can also expand Bessel function  $\mathcal{I}_0(x) \approx 1 - x^2/4$ . As the result we get the differential equation

$$\left( \ln \frac{T_{c0}}{T} - \psi \left( \frac{1}{2} + \frac{1}{4\pi\tau T} \right) + \psi \left( \frac{1}{2} \right) \right) \Delta(x) = -\frac{C}{2} \frac{I(\alpha)}{I(\alpha)} \left( \frac{v_F}{2\pi T} \right)^2 \Delta''(x) + I(\alpha) \left( \frac{t\omega_{c2}(T)x}{\pi v_F T} \right)^2 \Delta(x), \quad (40)$$

where  $\alpha = (2\pi T\tau)^{-1}$ ,

$$I(\alpha) = \int_0^\infty \frac{z^2 dz}{\sinh z} \exp(-\alpha z) = 4 \sum_{n=0}^\infty \frac{1}{(2n+1+\alpha)^3}, \quad (41)$$

$$C_\psi = \int_0^\pi \frac{d\phi}{\pi} \psi^*(\phi) \psi(\phi) \sin^2 \phi. \quad (42)$$

In pure case  $\alpha \approx \alpha_c = (2\pi T_c \tau)^{-1} \ll 1$  the inequality (38) is valid only in vicinity of the critical temperature. Putting  $T = T_c$  in the right hand side and taking its lowest eigen value we obtain

$$\ln \frac{T_{c0}}{T} - \psi \left( \frac{1}{2} + \frac{1}{4\pi\tau T} \right) + \psi \left( \frac{1}{2} \right) = \frac{\sqrt{C_\psi} I(\alpha_c) t \omega_{c2}(T)}{2\sqrt{2}\pi^2 T_c^2}. \quad (43)$$

Summing this equation with equation (32) and leaving only linear on  $T - T_c$  and on the impurity concentration terms we get

$$\omega_{c2}(T) = \frac{ev_F d}{c} H_{c2}(T) = \frac{4\sqrt{2}\pi^2}{7\zeta(3)\sqrt{C_\psi} t} \left( T_{c0} - \beta \frac{\pi}{8\tau} \right) (T_c - T). \quad (44)$$

Here the coefficient

$$\beta = 2 - \frac{90\zeta(4)}{7\pi^2\zeta(3)} \approx 0.83, \quad (45)$$

shows that, the slop of  $H_{c2}(T)$  at  $T = T_c$  decreases with the increase of the impurity concentration somewhat slower than  $T_c$  itself (see eqn. (33)).

The equation (36) does not contain any divergency of  $H_{c2}(T)$  and the expression (44) which is valid in Ginzburg-Landau region can be used at arbitrary temperature as the estimate of upper critical field from above. Hence, to establish the limits of a sample purity, at which the equation (36) works, one may substitute (44) at zero temperature into the inequality (35). Omitting the numerical factor of the order of unity we have

$$l < \frac{t}{T_c} \xi_{ab}, \quad (46)$$

where  $\xi_{ab} = v_F/2\pi T_c$  is the basal plane coherence length. We see, that there is the good reserve in sample purity in the limits of which one can not expect low temperature divergency of the upper critical field. In the  $Sr_2RuO_4$  the mean free path should be approximately 10 times larger than the basal plane coherence length  $\xi_0$  to go out limit (46).

Let us consider now the dirty case:  $T_c \ll T_{c0}$ ,  $\alpha \gg 1$  and  $I(\alpha) \approx \alpha^{-2}$  allowing analytical solution for  $H_{c2}(T)$  at arbitrary temperature. Taking the lowest eigen value of the equation (40) we get

$$\ln \frac{T_{c0}}{T} - \psi \left( \frac{1}{2} + \frac{1}{4\pi\tau T} \right) + \psi \left( \frac{1}{2} \right) = \sqrt{2C_\psi} \tau^2 t \omega_{c2}(T). \quad (47)$$

Summing of this equation with equation (32) yields

$$\omega_{c2}(T) = \frac{\ln \frac{T_c}{T} - \psi \left( \frac{1}{2} + \frac{1}{4\pi\tau T} \right) + \psi \left( \frac{1}{2} + \frac{1}{4\pi\tau T_c} \right)}{\sqrt{2C_\psi} \tau^2 t}. \quad (48)$$

This expression is correct at any temperature. One can rewrite it approximatively in more simple form

$$\omega_{c2}(T) = \frac{\sqrt{2}\pi^2}{3\sqrt{C_\psi}t} (T_c^2 - T^2), \quad (49)$$

where

$$T_c = \frac{1}{\pi\tau} \left( \frac{3}{2} \ln \frac{\pi T_{c0}\tau}{\gamma} \right)^{1/2}. \quad (50)$$

#### IV. CONCLUSION

The system of linear integral equations for the order parameter of conventional and unconventional superconducting state in a layered crystals with impurities under magnetic field parallel to the conducting layers is derived. It is shown that so long the purity of the samples does not exceed high enough level (46) there is no tendency to the low temperature divergency of the upper critical field. The analytical solution of the equations in the clean (Ginzburg-Landau region) and dirty (arbitrary temperature) limits are presented.

#### ACKNOWLEDGEMENTS

I express my best gratitudes to Dr. Manfred Sigrist and all the members of Condensed matter theory group at Yukawa Institute for Theoretical physics for their kind hospitality and interest to my work during my stay in Kyoto autumn 1999 where the significant part of this work have been completed.

I also indebted to Dr. Yoshiteru Maeno and his collaborators having stimulated my interest to the problem of upper critical field in layered superconductors.

I appreciate the valuable remarques of prof. M.Walker, prof. P.Nozieres and prof. Yu.A.Bychkov have resulted in the improvement in the initial text of the article.

- 
- <sup>1</sup> A.G.Lebed', K.Yamaji, Phys. Rev. Lett. **80**, 2697 (1998).
- <sup>2</sup> A.G.Lebed', Pis'ma Zh.Eksp. Teor.Fiz. **44**, 89 (1986) [JETP Lett.**44**, 114 (1986)].
- <sup>3</sup> T.Ishiguro, Talk presented on 20 anniversary Colloquium on Organic Superconductivity, December 7, 1999, Orsay, Journal de Physique IV **10** Pr3, Pr3-139 (2000).
- <sup>4</sup> P.M.Chaikin, Talk presented on 20 anniversary Colloquium on Organic Superconductivity, December 7, 1999, Orsay, unpublished; see also I.J.Lee, M.J.Naughton, G.M.Danner, P.M.Chaikin, Phys. Rev. Lett. **78**, 3555 (1997).
- <sup>5</sup> Y.Maeno, S.Nishizaki, Z.Q.Mao, Journ. Supercond.**12**, 535 (1999).
- <sup>6</sup> A.P.Mackenzie, Journ. Supercond.**12**, 543 (1999).
- <sup>7</sup> A.P.Mackenzie, R.K.W.Hasselwimmer, A.W.Tyler, G.G.Lonzarich, Y.Mory, S.Nishizaki, Y.Maeno, Phys. Rev. Lett. **80**, 161 (1998).
- <sup>8</sup> Z.Q.Mao, Y.Mory, Y.Maeno, Phys. Rev. B **60**, 610 (1999).
- <sup>9</sup> K.Ishida, H.Mukuda, Y.Kitaoka, Z.Q.Mao, Y.Mori, Y.Maeno, Preprint, Osaka University, October 1999.
- <sup>10</sup> K.Ishida, H.Mukuda, Y.Kitaoka, K.Asayama, Z.Q.Mao, Y.Mori, Y.Maeno, Nature, **396**, 658 (1998).
- <sup>11</sup> T.Akima, S.Nishizaki, Y.Maeno, Journ. Phys. Soc. Jap. **68**, 694 (1999).
- <sup>12</sup> K.Yoshida, Y.Maeno, S.Nishizaki, T.Fujita, Physica C **263**, 519 (1999).
- <sup>13</sup> E.Ohmichi, Y.Maeno, S.Nagai, Z.Q.Mao, M.A.Tanatar, T.Ishiguro, submitted to Phys. Rev. B, October 1999.
- <sup>14</sup> I.A.Lukyanchuk, V.P.Mineev, Zh. Eksp. Teor. Fiz. **93**, 2045 (1987) [Sov. Phys. JETP **66**, 1968 (1987)].
- <sup>15</sup> V.P.Mineev, K.V.Samokhin, "Introduction to unconventional superconductivity", Gordon and Breach Sc. Publ, 1999.
- <sup>16</sup> C.H.Choi, J.A.Sauls, Phys. Rev. B **48**, 13684 (1993)
- <sup>17</sup> Yu.A.Bychkov, ZhETF,**39**, 1401 (1960) [ Soviet Physics JETP, **12**, 977 (1960)].
- <sup>18</sup> Y.Hasegawa, K.Kishigi, M.Miyazaki, Journ. Supercond. **12**, 479 (1999).